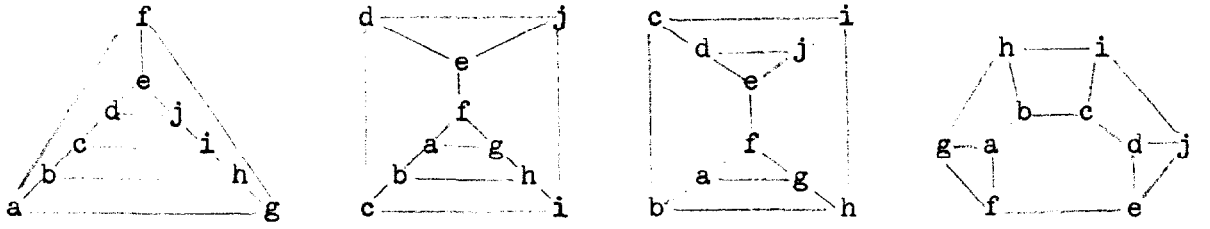
MAR 3 1 1965

1931 Golden Gate
San Francisco, Calif. 94115
March 30, 1965

Professor Joshua Lederberg
Stanford University School of Medicine
Palo Alto, California

Dear Professor Lederberg:

Thanks very much for your letter of March 26, the reprint of your very interesting paper and the two pages of Figures 1-7. To answer your postscript first, Rule 43 doesn't apply to 10A4A and 10A4B because they have no crossed bonds or shared bridges. Rule 30, however, gives identical notations for all four diagrams, 10A3, 10A4A, 10A4B and 10A6. The locant paths are as follows:



10A3 10A4A 10A4B 10A6

The notation is L634 B4 C4 D3 4ABCD JTJ for any of these representations of this structure. Wiswesser has shown this identity in another way by citing the pairs of connected locants that are not alphabetically consecutive. Here they are af, ag, bh, ci, dj, ej, and are identical for each representation.

This locant path produces the lowest sum for the fusion locants--Wiswesser's original conjecture--and this is still the most used consideration by far of Rule 30. The locant path is most easily found in 10A6 where the ring atoms that are shared by three cited rings (the multicyclic points) all appear in the interior of the planar representation and not in the peripheral uncited six-membered ring. Typically, the planar representation in which the peripheral ring is as large as possible is easiest to encode in this way. I have devoted considerable discussion to these transformations of alternate representations in the revision of the Wiswesser manual which I'm writing.

The largest effort of which I'm aware for converting Wiswesser notations to other forms is that of Drs. Franc Landee and Carl Bowman of The Dow Chemical Co. Since I'm their consultant I suppose I must be a bit careful about what I say, but they made public considerable information about their work at the American Chemical Society meeting in Philadelphia in April of last year. It has not been published, however. Among other things they have developed algorithms for converting the notation to atom connectivity tables and I believe they can manipulate these in various ways. I expect to see Dr. Bowman next week at the Detroit meeting of the American Chemical Society and perhaps after that I can answer your question in more detail.

I'd like very much to visit your computational system open house on April 19. I'm also looking for ard with great interest to hearing your talk at the Berkeley ACS meeting in April.

Sincerely,

Elbert G. Smith
Professor of Chemistry
Mills College